

Electron-phonon Interaction close to a Mott transition

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The effect of Holstein electron-phonon interaction on a Hubbard model close to a Mott-Hubbard transition at half-filling is investigated by means of Dynamical Mean-Field Theory. We observe a reduction of the effective mass that we interpret in terms of a reduced effective repulsion. When the repulsion is rescaled to take into account this effect, the quasiparticle low-energy features are unaffected by the electron-phonon interaction. Phonon features are only observed within the high-energy Hubbard bands. The lack of electron-phonon fingerprints in the quasiparticle physics can be explained interpreting the quasiparticle motion in terms of rare fast processes.

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Electron-phonon (e-ph) interaction is a key effect in solids, that gives rise to superconductivity, charge-density-waves and other important effects. While the physical phenomena caused by e-ph coupling in weakly correlated materials are reasonably well understood, much less is known about the role of e-ph coupling in strongly correlated materials, i.e., in compounds in which the short-range Coulomb repulsion is larger than the typical kinetic energy. This issue, besides its obvious general interest, has been strongly revived by recent experiments which suggest a role of lattice effects in the high-temperature superconducting cuprates (which are known to be strongly correlated compounds) [1], and by the realization that strong correlations are important in phonon-mediated superconductors as the fullerenes [2, 3].

The interplay between e-ph and electron-electron (e-e) interactions is quite a complicated problem, in which a variety of physical regimes and different phases can be realized. In the present paper we focus on the strongly correlated regime, in which the e-e interaction is assumed to be quite large, and the mobility of the electrons is strongly reduced. Our main concern is to understand whether and to which extent the e-ph coupling can still influence the electronic properties in this regime. We notice that the symmetry of the e-ph coupling is important in this regard: It has indeed been shown that a Jahn-Teller coupling, where the phonon variables are coupled with orbital and spin degrees of freedom is weakly affected by Hubbard repulsion U , whereas a Holstein coupling with the local charge is strongly suppressed [3, 4]. Nevertheless, even the Holstein coupling, if sizeable, can have a qualitative physical effect in a correlated material. For instance, it can induce phase separation close to the density-driven Mott transition [5]. A recent important contribution comes from the two-dimensional Quantum Monte Carlo study of Ref. [6], where a small U is found to suppresses the e-ph coupling at all electron and phonon momenta, while, in the strongly correlated regime, the forward-scattering amplitude due to e-ph processes sub-

stantially increases with U , leading to a non-monotonic behavior of the effective coupling.

In this work we consider again the simplest case of the Holstein interaction, whose formal simplicity allows for extensive systematic studies. Our Hamiltonian reads

$$H = -t \sum_{\langle i,j \rangle, \sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - g \sum_i n_i (a_i + a_i^\dagger) + \omega_0 \sum_i a_i^\dagger a_i, \quad (1)$$

where $c_{i,\sigma}$ ($c_{i,\sigma}^\dagger$) and a_i (a_i^\dagger) are, respectively, destruction (creation) operators for fermions with spin σ and for local vibrations of frequency ω_0 on site i , t is the hopping amplitude, U is the local Hubbard repulsion and g is an e-ph coupling. Despite its simplified character, the Hubbard-Holstein model is expected to display a complicated phase diagram as a function of its parameters, the correlation strength U/D (D is the electronic half-bandwidth), the e-ph coupling $\lambda = 2g^2/\omega_0 D$, the adiabatic ratio ω_0/D and the density n [5, 7, 8]. As notable examples, this model presents the physics of the Mott transition when the Hubbard repulsion is the most important scale [9], a crossover to polaronic carriers or a bipolaronic metal-insulator transition for small U and large λ [7, 10], and it is expected to be unstable toward superconductivity, charge-density waves and antiferromagnetism in different regions of the phase diagrams [11]. To gain physical insight into some aspects of this phase diagram, it is necessary to fix some parameters, and put ourselves in a given regime. As we have said, we investigate the strongly correlated metallic region, close to the Mott transition at half-filling. Our analysis is therefore relevant for metallic phases of correlated materials, such as the doped cuprates.

We solve the model by means of Dynamical Mean-Field Theory (DMFT), which has emerged as one of the most reliable tools from the analysis of both correlated materials, and e-ph interactions. The method maps the lattice model onto a local theory which still retains full quantum dynamics, and it is therefore expected to be quite accurate for models with local interactions, such as (1). The

DMFT solution is enforced by solving the local dynamical theory and imposing a self-consistency condition [9]. The local problem is equivalent to an Anderson-Holstein impurity model[12] which has to be solved with some tool. In our work we use exact diagonalization [13], truncating the infinite phonon Hilbert space allowing up to N_{max} phonon states (ranging from 20 to 40), and using $N_b = 9$ sites in the conduction bath.

DMFT has been extensively used to study the half-filled Hubbard model, showing that, in the metallic region close to the Mott transition, the spectral function presents three features: the high-energy Hubbard bands at energy $\pm U/2$ and a narrow resonance at the Fermi level, whose width is proportional to the quasiparticle residue $Z = (1 - \partial\Sigma(\omega)/\partial\omega|_{\omega=0})^{-1}$, a quantity which decreases for increasing U and vanishes at the Mott transition. Due to the momentum independence of the self-energy, Z is also the inverse of the effective mass $Z = m/m^*$. On general grounds, we can expect two main effects of e-ph coupling starting from the situation described above. The first is a reduction of Z (equivalent to an enhancement of the effective mass). This effect is responsible for the polaron crossover for weak repulsion. The second effect is a phonon-mediated retarded attraction between electrons with opposite spins, which opposes the Hubbard repulsion leading to an effective dynamical interaction $U_{eff}(\omega) = U - \frac{2g^2\omega_0}{\omega_0^2 - \omega^2}$. In the antiadiabatic limit $\omega_0 \rightarrow \infty$ the attraction becomes static and equals the bipolaronic binding energy $2g^2/\omega_0$. While the first effect opposes to the electronic motion, the second effect instead favors the motion by screening the Hubbard repulsion and leads to an enhancement of Z (at least as far as $U > 2g^2/\omega_0$). The overall effect of the e-ph coupling on the correlated metallic phase is therefore hard to predict on intuitive grounds.

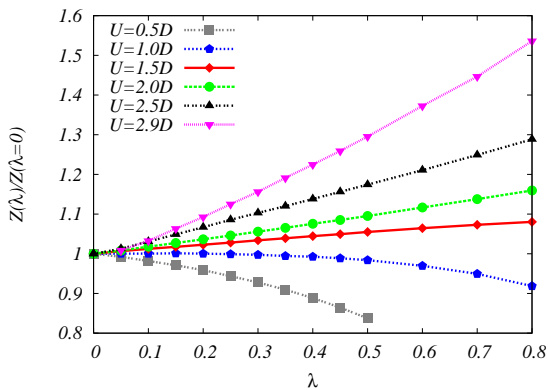


FIG. 1: (Color online) Effect of e-ph interaction on the quasiparticle weight Z . The ratio $Z(\lambda, U)/Z(0, U)$ is shown for different values of U and $\omega_0 = 0.2D$.

The DMFT study of model (1) helps us in understanding which of the two effects prevails. In Fig. 1 we report

the quasiparticle weight Z as a function of λ for different values of U/D for the half-filled Hubbard-Holstein model in the relatively adiabatic regime $\omega_0/D = 0.2$. In the absence of Hubbard repulsion, the effect of the e-ph coupling is quite naturally to increase the electron effective mass, and decrease Z , eventually reaching the bipolaronic metal-insulator transition [10]. Then we turn on the Hubbard repulsion, and plot the ratio $Z(U, \lambda)/Z(U, 0)$, in order to disentangle the effect of the e-ph interaction. While $Z(U, \lambda)$ is a decreasing function of U for each λ , the above ratio displays a richer behavior. Increasing the value of U , the effect of the e-ph interaction becomes weaker, until a value of $U \simeq 1.5D$ is reached, for which the e-ph coupling has the surprising effect to increase Z (reduce the effective mass), in agreement with the results found with a Numerical Renormalization Group solution of DMFT in Ref.7. This naively surprising result can be attributed, in light of the previous discussion, to the reduction of the effective repulsion, which prevails over the polaronic renormalization of the hopping. In the following we empirically determine an effective static repulsion $U_{eff}(U, \lambda, \omega_0)$, as the value of U for which a pure Hubbard model has the same Z as the full Hubbard-Holstein model. Since in the antiadiabatic limit $U_{eff} = U - \lambda D$, we try to parameterize the effective repulsion as $U_{eff} = U - \eta \lambda D$, where η is a dimensionless free parameter that we determine by fitting directly $Z(U, \lambda)$ with this functional form.

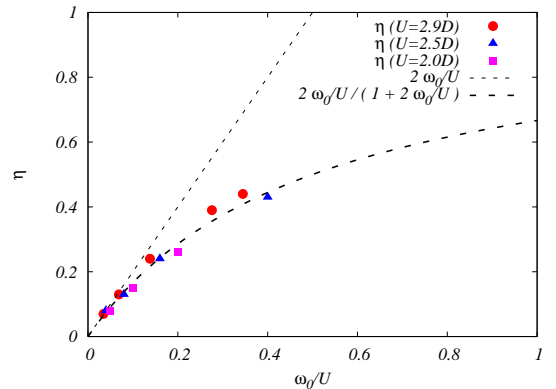


FIG. 2: (Color online) The coefficient η which measures the effective reduction of the Hubbard repulsion according to $U_{eff} = U - \eta \lambda D$, plotted as a function of ω_0/U . Different symbols refer to different values of U . The values of λ used for the fitting procedure described in the text, range typically from 0 to 1.

Computing η for different values of U and ω_0 , we find the behavior shown in Fig. 2. For relatively small ω_0/U , we find that η has a linear behavior in ω_0/U , and bends down for larger phonon frequency closely following the functional form $\eta = 2\omega_0/U / (1 + 2\omega_0/U)$ and eventually reaching the asymptotic value $\eta = 1$. We will see in the

following that this functional form can be derived from an expansion of the effective Kondo coupling[14].

The analysis of the quasiparticle weight suggests that the effect of e-ph interaction on the strongly correlated metallic phase of the Hubbard model is a partial screening of the repulsion, and the degree of screening is controlled by ω_0/U when this quantity is not too large. This latter factor contains the information about the lattice dynamics in an effective way. Of course, at this level, this result could sound of little physical significance, since it basically arises by a simple fit procedure. Nonetheless, Z also measures the width and weight of the low-energy feature in the single-particle spectral function. Thus, it is tempting to compare the spectral function for the Holstein model with the correspondent quantity for the equivalent Hubbard model with reduced repulsion. As far as $U \gg \omega_0$, we find that the low-energy part of the spectrum is basically identical in the two models, while differences develop in the high-energy part, where phonon satellites at energies of the order ω_0 appear in the system coupled to phonons. This can be seen in Fig.3, where the spectra for three different cases (see caption) are shown. Moreover, even if the effect of phonons is visible in the high-energy Hubbard bands, their position is more or less coincident in the Hubbard-Holstein model and in the effective Hubbard model. This is quite surprising, since the rescaling of U has been derived only by requiring the same value for the quasiparticle weight.

This findings strongly suggest that our reduction of the dynamical effective interaction to a static quantity is not a mere fitting, but it unveils some basic physics. We can gain some understanding of this scenario by exploiting the fact that the quasiparticle peak is associated within DMFT to a Kondo effect in the impurity model. It has been recently pointed out that, at the leading order in $1/U$, the Kondo coupling J_K is only weakly affected by e-ph coupling [14]. This result is closely related to a previous calculation addressing the effect of e-ph interaction on the superexchange coupling in a Hubbard model [15]. In both cases, the coupling (Kondo or antiferromagnetic) arises in fact, at the leading order in $1/U$, from virtual processes in which doubly occupied sites are created, with and energy cost of order U . In the presence of an e-ph coupling, the intermediate states can have an arbitrary number of phonons, but, in the limit in which $\omega_0 \ll U$, the corrections are small, and J_K is not substantially affected. More specifically, summing the contributions from all the states with different phonon occupation (see, e.g., Eq.(8) of Ref.14), one obtains a small correction of J_K given, at first order in λ_0/U , by

$$\frac{J_K(\lambda)}{J_K(0)} \simeq 1 + \frac{\lambda D}{U} \frac{\frac{2\omega_0}{U}}{1 + \frac{2\omega_0}{U}}, \quad (2)$$

which at first order in ω_0/U becomes $J_K(\lambda)/J_K(0) \simeq 1 + 2\omega_0\lambda D/U^2 = 1 + 4g^2/U^2$. Eq. (2) determines

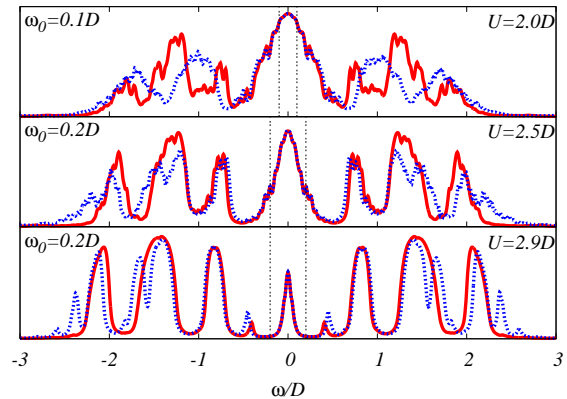


FIG. 3: (Color online) The electron spectral function for the Hubbard-Holstein model (dashed line), compared with a pure Hubbard model with $U = U_{eff} = U - \eta\lambda D$ (solid line), for different values of U and ω_0 (the dot-dashed vertical line indicates ω_0). In the two upper panels we take $\lambda = 1$, in the lowest $\lambda = 0.5$.

an effective static U for the Kondo problem given by $U_{eff}^K = U - \eta^K \lambda D$, with $\eta^K = (2\omega_0/U)/(1+2\omega_0/U)$. The agreement between the η extracted from DMFT and this prediction is evident from Fig. 2. This provides a strong physical interpretation of our previous finding about the effective U giving rise to the renormalization of the quasiparticle weight for small ω_0/U , for which we obtain the same dependence (see Fig. 2). Indeed within DMFT, the formation of the quasiparticle peak can be associated to a Kondo effect, which may in turn be described as arising from virtual processes of the same kind as the ones that lead to the Kondo coupling. But for the overall rescaling of U_{eff} , looking in detail to the phonon-induced modifications of the low-energy spectrum (the Kondo resonance in the single-impurity language) we found that these modifications are quantitatively extremely small and almost invisible on the resolution scale of Fig.3 [16].

The picture that emerges from the previous arguments can be summarized as follows: Quasiparticle motion arises from virtual processes in which doubly occupied sites are created. Obviously, these processes are not so frequent, since the energy scale involved is large, but they are extremely rapid (the associated time scale is $\propto 1/U$), and consequently are poorly affected by phonon excitations with a characteristic time scale $1/\omega_0 \gg 1/U$. When the phonon frequency is small with respect to U , the phonon degrees are frozen during the virtual excitation processes. Therefore, despite the overall electron motion is quite slow due to the small number of virtual processes (which is reflected by the large effective mass), the e-ph interaction has no major effect except for a slight reduction of the total static repulsion.

Finally, we come to some recent experimental evidences of phononic effects in the strongly correlated

cuprate superconductors. It must be noted that our results refer to the half-filled case for U smaller than the Mott transition point, while the experiments obviously refer to a doped system most likely with a larger U . Nevertheless it is tempting to assume that also in the U vs. doping region, relevant for the cuprates, the main low-energy effect of phonons is a small down-shift of the repulsion, that will be of no relevance when U is appreciably larger than its value at the Mott transition point. Our main finding of a completely different effect of e-ph coupling on the low-energy part of the spectrum with respect to the high-energy region, may provide an explanation of the observation of e-ph interaction in the high-energy branch of the ARPES spectra, in contrast to the weak effect on the low-energy part, as observed in recent isotope effect measurements [17]. On the other hand, if the system is close to the Mott transition, a slight modification of $U_{eff} = U - 2\omega_0\lambda D/U$ through the variation of ω_0 can significantly change the effective mass, leading to important isotope effects, affecting the penetration depth, as found in various underdoped samples [18]. A more detailed analysis of the evolution of the isotope effects in the full U vs. doping diagram is worth being carried out to provide a more reliable comparison with the available experiments.

A main limitation of our work, in light of previous studies of the problem of e-ph interactions, is the inability of DMFT to capture the momentum dependence of the phonon vertex. Even for the Holstein model, in which the bare coupling is local, i.e., momentum independent, it has indeed been shown that correlation effects tend to favor small exchanged momenta (forward) scattering [6, 19]. In this perspective, our DMFT results indicating that the local effects of the Holstein coupling are strongly renormalized down by correlations, allow to conclude that “standard” features of the e-ph coupling (polaron crossover, ordinary BCS pairing) are negatively influenced by correlation, while non-standard effects related to the strong forward scattering can survive and even get enhanced. In other words, if any Holstein-like e-ph interaction turns out to be relevant in strongly correlated materials, it must display anomalous features associated to the relevance of forward scattering and consequently requires a wider framework than ordinary Migdal-Eliashberg theory. On the other hand, the strong reduction by U does not apply to e-ph coupling involving degrees of freedom non competing with local charge fluctuations. This is the case for the Jahn-Teller coupling considered in Ref.[3], where the phonon-mediated pairing is indeed enhanced by strong correlations.

We have studied the half-filled Hubbard-Holstein model in the strongly correlated regime, where correlation effects are most important and determine a clear separation between low-energy quasiparticle features and “insulating” Hubbard bands. In this regime, we find that e-ph interaction has basically no effect on the quasi-

particle features as long as the Hubbard repulsion is suitably rescaled. An effective static repulsion $U_{eff} = U - 2\omega_0\lambda D/U$ in fact reproduces the low-energy features of the Hubbard-Holstein model using a simple Hubbard model. On the other hand, the high-energy Hubbard bands display phononic features that can not be found in an effective purely electronic model, even if the same scaling of U also reproduces the correct position of the bands. The “protection” of the low-energy physics with respect to e-ph interactions is provided by the (small) effect of lattice coupling on the Kondo coupling and on the resonance shape. We understand this result in terms of freezing of phonons on the time-scale relevant to virtual processes underlying the quasiparticle motion.

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- [1] A. Lanzara, *et al.*, Nature **412**, 510 (2001); M. d’Astuto, *et al.*, Phys. Rev. Lett. **88**, 167002 (2002). L. Pintschovius and W. Reichardt, in *Neutron Scattering in Layered Copper-Oxide Superconductors*, edited by A. Furrer, Physics and Chemistry of Materials with Low Dimensional Structures Vol. 20 (Kluwer Academic, Dordrecht, 1998), p. 165
 - [2] O. Gunnarsson, E. Koch and R. M. Martin Phys. Rev. B **54**, R11026 (1996); P. Durand, *et al.*, Nature Materials **2**, 605 (2003).
 - [3] M. Capone, *et al.*, Science, **296**, 2364 (2002).
 - [4] J. E. Han, O. Gunnarsson and V. H. Crespi, Phys. Rev. Lett. **90**, 167006 (2003).
 - [5] M. Capone, *et al.*, Phys. Rev. Lett. **92**, 106401 (2004).
 - [6] Z. B. Huang, W. Hanke, E. Arrigoni and D. J. Scalapino, Phys. Rev. B **68**, 220507(R) (2003).
 - [7] W. Koller, *et al.* Europhys. Lett. **66**, 559 (2004); W. Koller, D. Meyer and A. C. Hewson, Phys. Rev. B **70**, 155103 (2004).
 - [8] G. S. Jeon, *et al.*, Phys. Rev. B **70**, 125114 (2004).
 - [9] A. Georges, *et al.*, Rev. Mod. Phys. **68** 13 (1996).
 - [10] M. Capone and S. Ciuchi, Phys. Rev. Lett. **91**, 186405 (2003)
 - [11] J. K. Freericks and M. Jarrell, Phys. Rev. Lett. **75**, 2570 (1995); H. Fehske, *et al.*, Phys. Rev. B **69**, 165115 (2004);
 - [12] A.C. Hewson and D. Meyer, J. Phys.: Condens. Matter **14**, 427 (2002)
 - [13] M. Caffarel and W. Krauth, Phys. Rev. Lett. **72**, 1545 (1994).
 - [14] P.S. Cornaglia, H. Ness and D.R. Grempel, Phys. Rev. Lett. **93**, 147201 (2004).
 - [15] W. Stephan, *et al.*, Phys. Lett. A **227**, 120 (1997).
 - [16] From an analytic solution of the two-site case ($N_b = 1$) we find that these modifications scale with a coupling $(\omega_0/U)\lambda \ll \lambda$.
 - [17] H.-H. Gweon, *et al.*, Nature **430**, 187 (2004).
 - [18] G. M. Zhao, *et al.*, Nature (London) **385**, 236 (1997); R. Khasanov, *et al.*, Phys. Rev. Lett. **92**, 057602 (2004). For

- a review on isotope effects in cuprates see, e.g. J.P. Franck *Physical Properties of High Temperature superconductors* Vol. IV, edited by D.M. Ginsburg (World Scientific, 1994)
- [19] M. Grilli and C. Castellani, Phys. Rev. B **50**, 16880 (1994); M. L. Kulić, Phys. Rep. **338**, 1 (2000) and references therein; E. Cappelluti, B. Cerruti and L. Pietronero, Phys. Rev. B **69**, 161101(R) (2004).